

Signature of superconducting states in cubic crystal without inversion symmetry

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Abstract

The effects of absence of inversion symmetry on superconducting states are investigated theoretically. In particular we focus on the noncentrosymmetric compounds which have the cubic symmetry O like $\text{Li}_2\text{Pt}_3\text{B}$. An appropriate and isotropic spin-orbital interaction is added in the Hamiltonian and it acts like a magnetic monopole in the momentum space. The consequent pairing wavefunction has an additional triplet component in the pseudospin space, and a Zeeman magnetic field \mathbf{B} can induce a collinear supercurrent \mathbf{J} with a coefficient $\kappa(T)$. The effects of anisotropy embedded in the cubic symmetry and the nodal superconducting gap function on $\kappa(T)$ are also considered. From the macroscopic perspectives, the pair of mutually induced \mathbf{J} and magnetization \mathbf{M} can affect the distribution of magnetic field in such noncentrosymmetric superconductors, which is studied through solving the Maxwell equation in the Meissner geometry as well as the case of a single vortex line. In both cases, magnetic fields perpendicular to the external ones emerge as a signature of the broken symmetry.

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I. INTRODUCTION

The family of fermion superfluid, which includes the classes of conventional superconductor, helium-3 superfluid, and cuprate superconductor, has been one of the most frontier subjects in condensed matter physics. According to the parity symmetry of their pairing wavefunction,¹ the above classes can be labeled as *s*-wave, *p*-wave, and *d*-wave superfluid respectively and each has distinct thermodynamic and transport properties. In a system without inversion symmetry, this classification is however invalid, and the system is expected to simultaneously possess the properties belonging to distinct classes. Symmetry of the pairing wavefunctions as well as the gap functions are the immediate question. Theoretical studies based on the addition of a spin-orbital interaction in the Hamiltonian predict the Cooper pair to be a mixed state of singlet and triplet in pseudo-spin space,² which can lead to a non-vanishing spin susceptibility at zero temperature.^{2,3,4} Besides, the nodal gap structure has been investigated experimentally^{5,6,7,8} on two typical superconducting compounds, CePt₃Si and Li₂Pt₃B,^{9,10} which have the point group symmetries of C_{4v} and O , respectively.

On the other hand, the spin-orbital interaction also provides a correlation between the electric and magnetic degrees of freedom within the Fermi sea, connecting with the magnetic properties of the superconducting state in a subtle way. For example, a net polarization of spins can be induced by a shift of momenta distribution or vice versa in the superconducting state.^{3,11,12} In other words, the supercurrent and magnetization can be mutually induced. Therefore, the macroscopic distributions of current and magnetic field in the superconducting state can also be used to probe the effect of lacking inversion symmetry.^{13,14,15,16} One should note that the form of spin-orbital interaction must vary with the background crystals of different point group symmetry. Consequently the magnetic properties pertaining to superconducting CePt₃Si and Li₂Pt₃B are expected to be quite different. However, almost all the previous theoretical studies are based on the symmetry of C_{4v} which allows the Rashba form of spin-orbital interaction.

In this paper we focus on the magnetic properties pertaining to the compounds with crystal symmetry of O , such as Li₂Pt₃B. The starting point is to write down an appropriate spin-orbital interaction which turns out to act like a magnetic monopole in momentum space in this case. For simplicity we first consider the case of isotropic Fermi surface and pairing gap. The supercurrent \mathbf{J} is found to have a component parallel to the applied Zeeman

magnetic field \mathbf{B} and the proportional constant κ is obtained by the linear response theory. For macroscopic studies, we employ the Maxwell equation to investigate the distribution of magnetic field in the Meissner geometry and the case of a single vortex line. Lastly, we also consider the effects of anisotropy embedded in the cubic symmetry which causes a power-law dependence of $\kappa(T)$ for very low temperature due to the appearance of line nodes of superconducting gap functions.

II. MICROSCOPIC DERIVATION OF SUPERCURRENT INDUCED BY A ZEE-MAN FIELD

The goal of this section is to obtain an expression for the supercurrent induced by a Zeeman magnetic field in the bulk superconductor without inversion symmetry. We first consider the normal state. The lack of inversion symmetry is manifested itself by the spin-orbital interaction in the Hamiltonian $H = \sum_{\mathbf{p}} (H_{\mathbf{p}})_{\alpha\beta} a_{\mathbf{p}\alpha}^\dagger a_{\mathbf{p}\beta}$, in which the operator is given by,

$$H_{\mathbf{p}} = \frac{p^2}{2m} - E_F - \vec{h}_{\mathbf{p}} \cdot \vec{\sigma}, \quad (1)$$

and $a_{\mathbf{p}\alpha}$ are the second-quantized operators for electron of momentum \mathbf{p} and spin polarization $\alpha = \{\uparrow\downarrow\}$ is along the z axis in the laboratory frame. For convenience we write $\xi_{\mathbf{p}} = p^2/2m - E_f$. Note that the spin-orbital interaction is characterized by the parity-breaking inner product consisting of a parity-odd $\vec{h}_{\mathbf{p}} = -\vec{h}_{-\mathbf{p}}$ and the spin $\vec{\sigma}$ which is invariant under spatial inversion. It is convenient to work in the helicity basis (labelled by $\uparrow\downarrow$) in which the operator $\vec{h}_{\mathbf{p}} \cdot \vec{\sigma}$ is diagonal, that is,

$$\hat{h}_{\mathbf{p}} \cdot \vec{\sigma} |\mathbf{p} \uparrow\downarrow\rangle = \pm |\mathbf{p} \uparrow\downarrow\rangle. \quad (2)$$

The eigenvalues of $H_{\mathbf{p}}$ are thus given by $\epsilon_{\mathbf{p}}^\pm = \xi_{\mathbf{p}} \mp h_{\mathbf{p}}$ for positive \uparrow and negative \downarrow helicity, respectively. Hence the degenerate spectrum is split into two branches \pm in the presence of the spin-orbital interaction. The transformation between the helicity basis $\uparrow\downarrow$ and the laboratory frame basis $\uparrow\downarrow$ are given by the unitary operator $U_{\mathbf{p}} = \exp(-\frac{i}{2} \hat{\mathbf{k}} \cdot \vec{\sigma} \theta_{\mathbf{p}})$ which rotate the z axis by an angle of $\theta_{\mathbf{p}}$ around the axis of $\mathbf{k} = \mathbf{z} \times \hat{h}_{\mathbf{p}}$. More explicitly the matrix form of $U_{\mathbf{p}}$ can be written down in terms of the coordinate of $\hat{h}_{\mathbf{p}}$, namely,

$$U_{\mathbf{p}} = \begin{pmatrix} \cos \frac{\theta_{\mathbf{p}}}{2} & -e^{-i\phi_{\mathbf{p}}} \sin \frac{\theta_{\mathbf{p}}}{2} \\ e^{i\phi_{\mathbf{p}}} \sin \frac{\theta_{\mathbf{p}}}{2} & \cos \frac{\theta_{\mathbf{p}}}{2} \end{pmatrix} \quad (3)$$

Next we include the pairing between two electrons of opposite momenta on the same branch. In the helicity basis, a general mean-field description for the pairing potential H_{Δ} can be written as

$$H_{\Delta} = \sum_{\mathbf{p}} \left[\Delta_{+}^{*}(\mathbf{p}) a_{-\mathbf{p}\uparrow} a_{\mathbf{p}\uparrow} + \Delta_{-}^{*}(\mathbf{p}) a_{-\mathbf{p}\downarrow} a_{\mathbf{p}\downarrow} + h.c. \right], \quad (4)$$

where the two gap functions Δ_{+} and Δ_{-} , representing the pairing order parameter on the two branches, are not identical in general. However, the above pairing Hamiltonian can, by performing the transformation U , be restored to the case of singlet whenever $\Delta_{\pm}(\mathbf{p}) = e^{\mp i\phi_{\mathbf{p}}} |\Delta|$. Now the Nambu representation for the full Hamiltonian H in the helicity basis can be written as

$$H = \sum_{\mathbf{p}} \begin{pmatrix} a_{\mathbf{p}\uparrow}^{\dagger} & a_{-\mathbf{p}\uparrow} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{p}} - h_{\mathbf{p}} & \Delta_{+} \\ \Delta_{+}^{*} & -\xi_{\mathbf{p}} + h_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} a_{\mathbf{p}\uparrow} \\ a_{-\mathbf{p}\uparrow}^{\dagger} \end{pmatrix} \\ + \begin{pmatrix} a_{\mathbf{p}\downarrow}^{\dagger} & a_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{p}} + h_{\mathbf{p}} & \Delta_{-} \\ \Delta_{-}^{*} & -\xi_{\mathbf{p}} - h_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} a_{\mathbf{p}\downarrow} \\ a_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix}. \quad (5)$$

In what follows we employ the method of Matsubara Green's functions.¹⁷ It is useful to introduce the Nambu spinor representations $\Psi_{\mathbf{p}}$ and $\tilde{\Psi}_{\mathbf{p}}$ for $\uparrow\downarrow$ and $\downarrow\uparrow$ basis, respectively

$$\tilde{\Psi}_{\mathbf{p}} = \begin{pmatrix} a_{\mathbf{p}\uparrow} \\ a_{\mathbf{p}\downarrow} \\ a_{-\mathbf{p}\uparrow}^{\dagger} \\ a_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix}, \quad \Psi_{\mathbf{p}} = \begin{pmatrix} a_{\mathbf{p}\uparrow} \\ a_{\mathbf{p}\downarrow} \\ a_{-\mathbf{p}\uparrow}^{\dagger} \\ a_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix}. \quad (6)$$

The Matsubara Green's functions \check{G} in the $\uparrow\downarrow$ basis are defined in a complex time-ordered manner as

$$G_{\alpha\beta}(\mathbf{p}, \tau) = -\langle T_{\tau} \Psi_{\mathbf{p}\alpha}(\tau) \Psi_{\mathbf{p}\beta}^{\dagger}(0) \rangle, \quad (7)$$

and in the matrix form is

$$\check{G} = \begin{pmatrix} \hat{g} & \hat{f} \\ \hat{\bar{f}} & \hat{\bar{g}} \end{pmatrix}, \quad (8)$$

where \hat{g} and \hat{f} are the matrix forms of the ordinary Green's functions and Gor'kov Green's functions. We note that the lower components have the properties $\hat{\bar{g}}(\mathbf{p}, \tau) = -\hat{g}^{tr}(-\mathbf{p}, -\tau)$ and $\hat{\bar{f}}(\mathbf{p}, \tau) = \hat{f}^\dagger(\mathbf{p}, -\tau)$. The Fourier transformation of G is given by

$$G_{\alpha\beta}(\mathbf{p}, \omega_n) = \frac{1}{\beta} \int_0^\beta d\tau e^{i\omega_n \tau} G_{\alpha\beta}(\mathbf{p}, \tau). \quad (9)$$

where $1/\beta$ is the temperature and the frequency $\omega_n = (2n + 1)\pi/\beta$ is restricted due to the Fermi statistics. It is easier to first obtain the Green's function $\check{\check{G}}$ by simply inverting the matrix $(i\omega_n - H)$ in the helicity basis. The desired \check{G} can be obtained by performing the rotation in the pseudospin space using the followings,

$$\hat{g}(\mathbf{p}) = U_{\mathbf{p}} \hat{\bar{g}} U_{\mathbf{p}}^\dagger, \quad (10)$$

$$\hat{f}(\mathbf{p}) = U_{\mathbf{p}} \hat{\bar{f}} U_{-\mathbf{p}}^{tr}, \quad (11)$$

where the transformation matrix $U_{-\mathbf{p}}$ for the opposite momentum is given by $U_{\mathbf{p}}(-i\sigma_y)e^{i\sigma_z\phi_{\mathbf{p}}}$. Using the property that $\sigma_y \vec{\sigma}^{tr} \sigma_y = -\vec{\sigma}$, the expression for the Green's function \check{G} can be obtained as follows,

$$\begin{aligned} \hat{g} &= \frac{1}{2} \left[(g_+ + g_-) + (g_+ - g_-) \hat{h}_{\mathbf{p}} \cdot \vec{\sigma} \right], \\ \hat{f} &= \frac{1}{2} \left[(f_+ + f_-) + (f_+ - f_-) \hat{h}_{\mathbf{p}} \cdot \vec{\sigma} \right] (i\sigma_y). \end{aligned} \quad (12)$$

where the scalar functions g_\pm and f_\pm are given below

$$\begin{aligned} g_\pm &= -\frac{i\omega_n + \epsilon_{\mathbf{p}}^\pm}{\omega_n^2 + \epsilon_{\mathbf{p}}^{\pm 2} + |\Delta_\pm|^2}, \\ f_\pm &= \frac{\Delta_\pm e^{\pm i\phi_{\mathbf{p}}}}{\omega_n^2 + \epsilon_{\mathbf{p}}^{\pm 2} + |\Delta_\pm|^2}. \end{aligned} \quad (13)$$

where we note that the previous condition for the pairing to recover the singlet is consistent with the condition for which the triplet component of Gor'kov Green's function vanishes in Eq. (12).

In what follows we use the linear response theory to calculate the supercurrent \mathbf{J} induced by an external Zeeman magnetic field \vec{b} . We express the Fourier-transformed current operator in terms of the Nambu spinor representation as

$$\vec{J}_{\mathbf{q}} = \sum_{\mathbf{p}} \Psi_{\mathbf{p}-\alpha}^{\dagger} (\vec{v}_{\mathbf{p}})_{\alpha\beta} \Psi_{\mathbf{p}+\beta}, \quad (14)$$

where the momentum $\mathbf{p}_{\pm} = \mathbf{p} \pm \frac{\mathbf{q}}{2}$, and the velocity operator $\mathbf{v}_{\mathbf{p}}$ associated with momentum \mathbf{p} is obtained by taking derivative of Hamiltonian with respect to \mathbf{p} , which gives an identical result with the previous studies,¹⁵

$$\check{\vec{v}}_{\mathbf{p}} = \begin{pmatrix} \frac{\mathbf{p}}{m} - \nabla_{\mathbf{p}} \vec{h}_{\mathbf{p}} \cdot \vec{\sigma} & 0 \\ 0 & \frac{\mathbf{p}}{m} + \nabla_{\mathbf{p}} \vec{h}_{\mathbf{p}} \cdot \vec{\sigma}^{tr} \end{pmatrix}. \quad (15)$$

The paramagnetic perturbation V resulting from the Zeeman magnetic field $\vec{b}(r)$ is $V = -\mu \int dr \vec{s}(r) \cdot \vec{b}(r)$, here the positive μ is the magnetic moment and $\vec{s}(r)$ denotes the local spin density. V can be represented in Fourier space as $V = -\mu \vec{s}_{\mathbf{q}} \cdot \vec{b}_{-\mathbf{q}}$ in which the Fourier-transformed spin density is given by

$$\vec{s}_{\mathbf{q}} = \sum_{\mathbf{p}} \Psi_{\mathbf{p}-\mathbf{q}/2}^{\dagger} \vec{\Sigma} \Psi_{\mathbf{p}+\mathbf{q}/2}, \quad (16)$$

where $\vec{\Sigma}$ is the spin operator for the Nambu spinor representation, given by

$$\check{\vec{\Sigma}} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma}^{tr} \end{pmatrix} \quad (17)$$

After some arrangement the current \vec{J} can be written down explicitly as:

$$\begin{aligned} \vec{J}(\mathbf{q}, i\omega_n) &= - \int_0^{\beta} d\tau e^{i\omega_n \tau} \langle T_{\tau} \vec{J}_{\mathbf{q}}^{\dagger}(\tau) \vec{s}_{\mathbf{q}}(0) \rangle \cdot (-\mu \vec{b}_{-\mathbf{q}}) \\ &= -\frac{\mu}{\beta} \sum_{\mathbf{p}} \sum_{\omega_m} \frac{1}{2} \text{Tr}' \left[\check{\vec{v}}_{\mathbf{p}} \check{G}(\mathbf{p}_-, i\omega_m) (\check{\vec{\Sigma}} \cdot \vec{b}_{-\mathbf{q}}) \check{G}(\mathbf{p}_+, i\omega_n + i\omega_m) \right], \end{aligned} \quad (18)$$

in which the symbol Tr' denotes taking trace over both the electron and hole sectors, and a factor of $\frac{1}{2}$ is added to avoid double counting.

III. MANIFESTATION OF ABSENCE OF INVERSION SYMMETRY

In this section we are going to demonstrate the manifestation of absence of inversion symmetry in this cubic superconductors from both microscopic and macroscopic perspectives. Starting from the general expression for supercurrent in Eq. (18), we investigate the static and homogeneous case, that is, the limits $\mathbf{q} \rightarrow 0$ and $\omega_n \rightarrow 0$ are taken. The resultant static current \mathbf{J} is collinear with the applied field, which can be written as

$$\mathbf{J} = -\kappa(T)\mathbf{B} \quad (19)$$

where the macroscopic magnetic field, or the magnetic induction is $\mathbf{B} = \vec{b}_0$. The appearance of this coefficient κ is an important signature of the lack of inversion symmetry. In Sec.III A κ is studied explicitly for a given isotropic $\vec{h}_{\mathbf{p}}$.

Sec.III B is devoted to the studies of macroscopic aspects, which deals with the interaction between the magnetic field and the nonvanishing pairing order parameter Δ . A crucial addition of Eq. (19) to the ordinary supercurrent and the corresponding magnetization are the key ingredients for understanding the new distribution of magnetic field. By the way, the expressions for \mathbf{J} and \mathbf{M} can be obtained by taking the derivatives of free energy as,¹⁴

$$\begin{aligned} \mathbf{J} &= 2 \frac{\delta F}{\delta \vec{q}}, \\ \mathbf{M} &= -\frac{\delta F}{\delta \mathbf{B}}, \end{aligned} \quad (20)$$

where the gauge-invariant phase gradient $\vec{q} = \hbar \nabla \varphi + \frac{2e}{c} \mathbf{A}$ and the free energy F contains an extra term of $-\frac{1}{2} \kappa \vec{q} \cdot \mathbf{B}$ representing the absence of inversion symmetry.¹⁴ More explicitly the above expressions can be written as

$$\frac{4\pi}{c} e \mathbf{J} = \frac{1}{\lambda^2} (\mathbf{A} + \frac{c\hbar}{2e} \nabla \varphi) - \frac{\delta}{\lambda^2} \mathbf{B}, \quad (21)$$

$$4\pi \mathbf{M} = \frac{\delta}{\lambda^2} (\mathbf{A} + \frac{c\hbar}{2e} \nabla \varphi). \quad (22)$$

λ denotes the London penetration length. The length parameter $\delta = \frac{4e\pi}{c} \kappa \lambda^2$ is introduced for later convenience. Note that we have taken the electronic charge to be $(-e)$.

A. Microscopic aspects

Now we consider the simplest case for which the spin orbital interaction is isotropic, and the gaps are identical for both branches and isotropic as well, that is,

$$\begin{aligned}\vec{h}_{\mathbf{p}} &= \alpha \mathbf{p}, \\ \Delta_+ &= \Delta_- = \Delta.\end{aligned}\tag{23}$$

The strength of spin-orbital interaction is characterized by the quantity α , which has the dimension of velocity and is weak in the sense that $\alpha/v_F \ll 1$. Here v_F denotes the Fermi velocity. Starting from Eq. (18), with some arrangements, the static current can be obtained by taking the limit $\mathbf{q} \rightarrow 0$ of the following expression,

$$\mathbf{J}_{\mathbf{q}} = -\frac{\mu}{\beta} \int_{-\infty}^{+\infty} d\xi \nu(\xi) \sum_{\omega_n} \sum_{\mu, \nu=\pm} Q_{\mu\nu} \frac{(i\omega_n + \epsilon_{\mathbf{p}_+}^\mu)(i\omega_n + \epsilon_{\mathbf{p}_-}^\nu) + \Delta^2}{(\omega_n^2 + \epsilon_{\mathbf{p}_+}^{\mu^2} + \Delta^2)(\omega_n^2 + \epsilon_{\mathbf{p}_-}^{\nu^2} + \Delta^2)},\tag{24}$$

where the matrix elements of Q represent the factors for intra-branch contributions, $\mu = \nu = \pm$, and the inter-branch ones, $\mu = -\nu$. Explicitly, Q in the matrix form can be written as

$$Q = \begin{pmatrix} \frac{1}{2}\vec{n} - \frac{1}{4}(\vec{l} + \vec{t}) & -\frac{1}{4}(\vec{l} - \vec{t}) \\ -\frac{1}{4}(\vec{l} - \vec{t}) & -\frac{1}{2}\vec{n} - \frac{1}{4}(\vec{l} + \vec{t}) \end{pmatrix},\tag{25}$$

where the three vectors are obtained after the operation of trace and solid-angle integration, namely,

$$\begin{aligned}\vec{n} &= \int \frac{d\Omega}{4\pi} \text{Tr}[\frac{\mathbf{p}}{m}(\vec{\sigma} \cdot \mathbf{B})(\hat{\mathbf{p}} \cdot \vec{\sigma})] = \frac{2}{3} \frac{\mathbf{p}}{m} \mathbf{B}, \\ \vec{l} &= \int \frac{d\Omega}{4\pi} \text{Tr}[\alpha \vec{\sigma}(\vec{\sigma} \cdot \mathbf{B})] = 2\alpha \mathbf{B}, \\ \vec{t} &= \int \frac{d\Omega}{4\pi} \text{Tr}[\alpha \vec{\sigma}(\hat{\mathbf{p}} \cdot \vec{\sigma})(\vec{\sigma} \cdot \mathbf{B})(\hat{\mathbf{p}} \cdot \vec{\sigma})] = -\frac{2}{3}\alpha \mathbf{B}.\end{aligned}\tag{26}$$

Note that the trace here is only taken over a two-by-two helicity space in contrast to the previous operation in Eq. (18). First we note that the static current in Eq. (24) is zero when the spin-orbital interaction is absent. For \vec{n} , \vec{l} and \vec{t} in Eq. (26), therefore, only the contributions up to first order α/v_F are relevant. Since the summation over ω_n will give a

singular integrant concentrated at the Fermi level, it is eligible to substitute the quantities p and $\nu(\xi)$ with their values at Fermi level and then move them out of the integral. However, the contributions from \vec{n} in the diagonal parts of Q must be taken care of because explicitly they are of zeroth order of α/v_F . Hence the implicit contributions from modification of Fermi momentum and density of states due to the spin-orbital interaction have to be taken into account. Namely, the Fermi momentum for each branch, $p_F^\pm = p_F(1 \pm \alpha/v_F)$, and also the density of states at Fermi level, $\nu^\pm = mp_F^\pm(1 \pm \alpha/v_F)$, should be used here. We also use the trick which enables performing the integration of energy first,¹⁸ and after some algebra the coefficient κ is obtained as

$$\frac{\kappa(T)}{\mu\alpha\nu(0)} = -\frac{4}{3} \left\{ \left[1 - \frac{\pi}{\beta} \sum_n \frac{\Delta^2}{(\omega_n^2 + \Delta^2)^{\frac{3}{2}}} \right] - \left[1 - \frac{\pi}{\beta} \sum_n \frac{1}{(\omega_n^2 + \Delta^2)^{\frac{1}{2}}} \frac{\Delta^2}{\omega_n^2 + \Delta^2 + (\alpha p_F)^2} \right] \right\}. \quad (27)$$

The term in first bracket is actually the Yoshida function $Y(\Delta, T)$, which is a universal function characterizing the single-particle excitation across the gap Δ at temperature T . For an isotropic gap and at low temperature $T/\Delta \ll 1$, the function Y is proportional to $\exp(-\Delta/T)$. The second bracket is identical to the first one when the spin-orbital interaction is absent. We denote this term by a function $y(\Delta, \alpha, T)$ to represent the excitations between two superconducting states separated by an energy of αp_F . Thus we can rewrite Eq. (27) as $\kappa = \frac{4}{3}\mu\alpha\nu(0)(y - Y)$. At zero temperature, the function y can be evaluated by replacing the summation over the Matsubara frequency by an integral, and for isotropic Δ and α this function is given by,

$$y(\Delta, \alpha, T = 0) = 1 - \frac{1}{2\theta} \frac{1}{\sqrt{1 + \theta^2}} \ln \left(1 + 2\theta^2 + 2\theta\sqrt{1 + \theta^2} \right), \quad (28)$$

where the number $\theta = \alpha p_F/\Delta$. For small θ , the function $y \sim \frac{2}{3}\theta^2$. For large θ , it is approximately $1 - \frac{\ln(2\theta)}{\theta^2}$. Both limits coincide with the previous predictions.^{2,12}

In addition, the intra-branch and inter-branch contributions can be respectively recognized as the Pauli and Van Vleck ones in the previous studies.¹² Therefore the induced current \mathbf{J} is absent as the Pauli and Van Vleck contributions cancel each other in the normal state in which $Y = y = 1$. On the other hand, the existence of such current relies on the fact that the Pauli paramagnetic contribution in the superconducting state is significantly suppressed while the Van Vleck one is only reduced by a small portion as long as $\Delta \ll \alpha p_F$.

Consequently one can easily infer that the net supercurrent always flows in opposite to the Pauli paramagnetic current.

B. Macroscopic aspects

Here the effect of lacking inversion symmetry on a macroscopic length scale is studied through solving the static Maxwell equation,

$$\nabla \times \mathbf{B} = 4\pi \nabla \times \mathbf{M} + \frac{4\pi}{c}(-e)\mathbf{J}, \quad (29)$$

Together with the current and magnetization given by Eq. (21) and (22), we are able to obtain an equation in terms of magnetic field \mathbf{B} only, namely,

$$\nabla \times \nabla \times \mathbf{B} = -\frac{1}{\lambda^2}\mathbf{B} + 2\frac{\delta}{\lambda^2}\nabla \times \mathbf{B}, \quad (30)$$

in which the last curl term is generated from $\nabla \times \mathbf{M}$ as well as the collinear supercurrent induced by \mathbf{B} . Hence, one can expect to observe a transverse component of the applied Zeeman field in such noncentrosymmetric superconductors.

Eq. (30) can be applied for studying the penetration of magnetic field in Meissner geometry. Explicitly, we can consider a cubic superconductor occupying the space for $z > 0$. It is more convenient to first consider a general field $B_x(z)\hat{x} + B_y(z)\hat{y}$ containing both x and y components. Consequently, the equation with which the general field satisfies is,

$$\frac{d^2}{dz^2}B_+(z) = \frac{1}{\lambda^2}B_+(z) - 2i\frac{\delta}{\lambda^2}\frac{d}{dz}B_+(z), \quad (31)$$

where B_+ stands for the linear combination $B_x + iB_y$. Defining $B_+(z = 0^+) = B_{\text{in},+}$, the field just inside the superconductor, the general solution is then given by,

$$B_+(z > 0) = B_{\text{in},+}e^{-\frac{z}{\lambda}\left(\sqrt{1-\frac{\delta^2}{\lambda^2}}+i\frac{\delta}{\lambda}\right)}, \quad (32)$$

which is identical to the previous results.¹³ So one can expect a slight increase of penetration depth by a factor of $1/\sqrt{1-\frac{\delta^2}{\lambda^2}}$ for such cubic superconductors in Meissner geometry. Besides, we note that the additional oscillation is a consequence of a parallel component of \mathbf{J} to \mathbf{B} .

The unknown $B_{\text{in},+}$ in Eq. (32) can be determined from the boundary condition $\mathbf{B}_{\text{ext}} = \mathbf{B}_{\text{in}} - 4\pi\mathbf{M}(z = 0^+)$, which requires the knowledge of magnetization \mathbf{M} , or equivalently the gauge-invariant \vec{q} . In fact \vec{q} can be obtained from integration of the relation $(-i)B_+(z) = dA_+(z)/dz$ with given boundary condition at infinity. We can assume the homogeneity for phase φ throughout the superconductor, which is indicative of vanishing \mathbf{A} at $z = \infty$ to ensure zero current there. Consequently the boundary condition at the surface can be shown to, up to first order of δ/λ , have the following form,

$$i\lambda B_{\text{ext},+} = A_{\text{in},+} . \quad (33)$$

A similar relation for B_- can be obtained from the above by taking complex conjugates on both sides.

If the external field is $\mathbf{B}_{\text{ext}} = B\hat{x}$, then $A_x(0^+) = 0$ as a result of Eq. (33). Consequently, $M_x(0^+) = 0$, which demonstrates that the parallel field is continuous across the surface. In fact, the magnetic field B_x and B_y inside the superconductor can be obtained by taking the real and imaginary parts of Eq. (32), respectively. Up to first order of δ/λ , the two components can be written as,

$$B_x = B \left[\cos \frac{\delta z}{\lambda^2} + \frac{\delta}{\lambda} \sin \frac{\delta z}{\lambda^2} \right] e^{-\frac{z}{\lambda}} , \quad (34)$$

$$B_y = B \left[\frac{\delta}{\lambda} \cos \frac{\delta z}{\lambda^2} - \sin \frac{\delta z}{\lambda^2} \right] e^{-\frac{z}{\lambda}} . \quad (35)$$

Along the direction of applied field, the field B_x penetrates into the superconductor with an additionally slow oscillation of period about $\lambda/\frac{\delta}{\lambda}$. On the other hand, $M_y(0^+)$ is finite due to the existence of finite flow velocity proportional to A_y at the interface. Hence a discontinuity for field B_y is generated at the interface,

$$\frac{B_{\text{in},y} - B_{\text{ext},y}}{B_{\text{ext},x}} = \frac{\delta}{\lambda} , \quad (36)$$

which is different from the previous prediction for inversion-broken superconductor of C_{4v} symmetry where the discontinuity happens to the parallel field across the interface.¹⁴ The functional form of B_y in Eq. (35) indicates that it has the largest magnitude $\frac{\delta}{\lambda}B$ at the surface, changes sign at $z \cong \lambda$ and then decays to zero while slowly oscillating. Furthermore,

the flux associated with the perpendicular B_y is zero. This is consistent with the conclusion drawn from Eq. (33) that $A_x = 0$ at the interface since both $A_x(z = \infty)$ and A_z are zero.

Eq. (30) can also be applied for studying a single vortex line as a macroscopic signature of lacking inversion symmetry. We consider the conventional case in which the vortex line is along the z axis, and the cylindrical coordinates are adopted here. The components of magnetic field are assumed to be $B_\phi(r)$ and $B_z(r)$ along the directions of $\hat{\phi}$ and \hat{z} , respectively. The z and ϕ components of Eq. (30) are given by,

$$\left[\frac{1}{r} \frac{d}{dr} \left(r \frac{d}{dr} \right) - \frac{1}{\lambda^2} \right] B_z(r) = -\tilde{\kappa} \frac{1}{\lambda} \frac{1}{r} \frac{d}{dr} (r B_\phi), \quad (37)$$

$$\left[\frac{d}{dr} \left(\frac{1}{r} \frac{d}{dr} r \right) - \frac{1}{\lambda^2} \right] B_\phi(r) = \tilde{\kappa} \frac{1}{\lambda} \frac{d}{dr} B_z, \quad (38)$$

where we denote the dimensionless number $\tilde{\kappa} = 2\delta/\lambda$ for convenience. We can therefore assume the following perturbation solutions,

$$B_z = B_z^{(0)} + \tilde{\kappa}^2 B_z^{(2)} + \dots, \quad (39)$$

$$B_\phi = \tilde{\kappa} B_\phi^{(1)} + \tilde{\kappa}^3 B_\phi^{(3)} + \dots. \quad (40)$$

The zeroth order solution $B_z^{(0)}$ of Eq. (37) is just the conventional single vortex line solution, given by $\frac{\Phi}{2\pi\lambda^2} K_0(r/\lambda)$ where Φ is a quantum of flux $\frac{\pi\hbar c}{e}$ and K_0 is the modified Bessel function of zeroth order. As can be seen in Eq. (38), now the transverse field B_ϕ emerges as a result of the nonzero source proportional to K_1 from the identity $K_0' = -K_1$. Up to the first order of $\tilde{\kappa}$, the transverse field can be written down in terms of the Green's function g_1 associated with Eq. (38).¹⁹ Defining the dimensionless variable x as r/λ , it can be expressed as,

$$\begin{aligned} B_\phi^{(1)}(x) / \frac{\Phi}{2\pi\lambda^2} &= \int_0^\infty x' dx' g_1(x, x') K_1(x'), \\ &= K_1(x) \int_0^x x' dx' I_1(x') K_1(x') + I_1(x) \int_x^\infty x' dx' [K_1(x')]^2, \end{aligned} \quad (41)$$

in which K_1 and I_1 are the modified Bessel functions of first order. The asymptotic behaviors of the transverse field distribution are,

$$B_\phi^{(1)}(x) \sim \left\{ \begin{array}{ll} \frac{x}{2} \ln \frac{1}{x} & , \ x \rightarrow 0 \\ \sqrt{\frac{\pi x}{8}} e^{-x} & , \ x \rightarrow \infty \end{array} \right\}. \quad (42)$$

Hence the transverse field increases from zero at the origin, reaches its maximum at a distance of order λ from the center and is followed by an exponential decay. The above extra magnetic fields non-collinear with the externally applied one can in principle be detected by observing the extra precession of polarized muons when their polarization is parallel to the external applied field. $\frac{\delta}{\lambda}$ for $\text{Li}_2\text{Pt}_3\text{B}$ is of order 10^{-3} using the spin-orbital splitting estimated by Lee and Pickett.²⁰

IV. ANISOTROPIC FERMI SURFACE AND LINE NODES OF GAP

In previous sections we demonstrate an induced supercurrent parallel to the external Zeeman field as a signature of lacking inversion symmetry in cubic superconductors. Actually the spin-orbital interaction appropriate for the point group O respects all but the elements connected to inversion in O_h . The odd-parity basis functions²¹ $\{p_x^n\hat{x} + p_y^n\hat{y} + p_z^n\hat{z}; n = 1, 3, 5\}$, in which the cubic symmetry is embedded, belonging to A_{1u} representation within O_h still can be used to construct the vectors $\vec{h}_{\mathbf{p}}$. Similarly, the general gap function respecting the cubic symmetry,

$$\hat{\Delta}(\mathbf{p}) = (\Delta_0(\mathbf{p}) + \vec{d}_{\mathbf{p}} \cdot \vec{\sigma})(i\sigma_y), \quad (43)$$

can have the component $\Delta_0(\mathbf{p})$ constructed from the even-parity basis functions belonging to A_{1g} representation while the vector function $\vec{d}_{\mathbf{p}}$, having identical symmetry properties of $\vec{h}_{\mathbf{p}}$, can be constructed from A_{1u} representation. Here both components can be nonzero since parity is no longer respected. An important feature of the gap function given in Eq. (43) is the possible appearance of zeros when the order parameters $\Delta_0(\mathbf{p})$ and $\vec{d}_{\mathbf{p}}$ can simultaneously be real after appropriate gauge transformations, which is true if the time-reversal symmetry is respected in the system. Consequently it is possible to realize the zeros of gap function when $|\vec{d}_{\mathbf{p}}|$ exceeds $|\Delta_0(\mathbf{p})|$ for some points on the Fermi surface. Gapless excitation can therefore exist in such superconductors by showing, for example, a power law temperature dependence of penetration depth.²²

In fact the nodal structure of gap function in the compound $\text{Li}_2\text{Pt}_3\text{B}$ was shown to be line nodes through the observation of linear temperature dependence in penetration depth for very low temperature.^{7,22} Here we shall investigate the effects of anisotropy and line nodes on the coefficient $\kappa(T)$ near zero temperature. Since we are only interested in the regime of very

weak Zeeman field, the anisotropy, which could result in some nonlinear field dependence for stronger field regime, has little qualitative effect here. Hence only the line nodes of gap function are relevant to the low temperature behavior of $\kappa(T)$. The intra-branch, or the Pauli, contributions of $\kappa(T)$ in Eq. (27) for the isotropic case can be generalized here by directly replacing the gaps Δ_{\pm} with $|\Delta_0| \pm |\vec{d}|$. As for the inter-branch contribution, the gaps on both branches are in fact much smaller than the separation αp_F in $\text{Li}_2\text{Pt}_3\text{B}$, which suggests little relevance of actual gap function this contribution. Moreover, even the appearance of zeros associated with the spin-orbital interaction $\alpha(\Omega)$ are also irrelevant to the T -dependence of this contribution at very low temperature as long as the zeros associated with α are not identical to those associated with the pairing gap.

We thus define a dimensionless quantity $\gamma(T) \equiv \frac{\kappa(0) - \kappa(T)}{\kappa(0)}$ to present the temperature dependence due to the line nodes at temperature close to zero. Furthermore, from previous arguments, only the intra-branch contributions associated with the pairing gap of $|\Delta_0| - |\vec{d}|$ is significant here. In addition, we are only interested in the effects due to the line nodes and take these parameters $\alpha(\Omega)$ and $v_F(\Omega)$ to be isotropic, which makes the evaluation easier and more accessible. Next the summation over ω_n in the function Y in Eq. (27) can be transformed into an integral of energy, which makes $\gamma(T)$ into the following form,

$$\gamma(T) = \int \frac{d\Omega}{4\pi} (\cos \theta)^2 \Delta_-^2(\hat{\Omega}) \int_0^\infty d\xi \left(\frac{1}{E^3} \frac{2}{e^{E/T} + 1} + \frac{1}{2E^2 T} \frac{1}{\cosh^2(E/2T)} \right), \quad (44)$$

where the Zeeman field is assumed to be along the z axis, and $\Delta_-(\hat{\Omega})$ denotes the gap functions of the direction $\hat{\Omega}$ on the Fermi surface, and $E = \sqrt{\xi^2 + \Delta_-^2(\hat{\Omega})}$. We note that the above integral vanishes for T is exactly zero since E is always positive for all ξ . Hence the contribution for T slightly larger than zero comes from integration around the solid angles Ω associated with the zeros of gap. By the cubic symmetry, we can infer that there are six sets of line nodes on the Fermi surface, which as a whole remain invariant under any cubic rotation. Hence the contributions from the six sets can be divided into $\gamma(T) = 2\gamma_{\parallel}(T) + 4\gamma_{\perp}(T)$, where γ_{\parallel} denotes that from the line nodes that are symmetrically distributed around the z axis, while γ_{\perp} denotes remaining sets that are around the x or y axis.

For a given set of line nodes, the gap function can be expanded around these zeros in the following manner,

$$\Delta_-(\hat{\Omega}) = \Delta'(\theta_c)(\theta - \theta_c), \quad (45)$$

which means the solid angel $\hat{\Omega} = (\theta, \phi)$ associated with the zeros can be parameterized as $(\theta_c(\phi), \phi)$ along the azimuthal direction. $\Delta'(\theta_c)$ denotes the slope of gap function along the direction of $\hat{\theta}$. Finally the linear temperature dependence can be extracted from $\gamma(T)$, and the following expression can be obtained if one extends the upper limit of θ integral to infinity.

$$\begin{pmatrix} \gamma_{\parallel}(T) \\ \gamma_{\perp}(T) \end{pmatrix} = \int \frac{d\phi}{2\pi} \begin{pmatrix} \cos^2 \theta_c \\ \sin^2 \theta_c \cos^2 \phi \end{pmatrix} \frac{T}{\Delta'(\theta_c)} \int_0^{\infty} \int_0^{\infty} x^2 dx dy \left(\frac{2}{r^3} \frac{1}{e^r + 1} + \frac{1}{2r^2} \frac{1}{\cosh^2(r/2)} \right), \quad (46)$$

in which $x = \theta \Delta'(\theta_c)/T$, $y = \xi/T$ and $r = \sqrt{x^2 + y^2}$. In terms of polar coordinate the integral is to give $\pi \ln 2$.

V. CONCLUSIONS

In this work we demonstrate an induced supercurrent parallel to the external Zeeman magnetic field utilizing the Green's function method. Besides, the induced supercurrent and the consequent magnetization modify the distribution of magnetic fields in the Meissner geometry as well as in the vortex line. Transverse magnetic fields are generated as a sign of breaking inversion symmetry in superconductors of point group symmetry O such as $\text{Li}_2\text{Pt}_3\text{B}$.

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